Absolute Remote Sensing

Forward models for Bayesian inference

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Outline

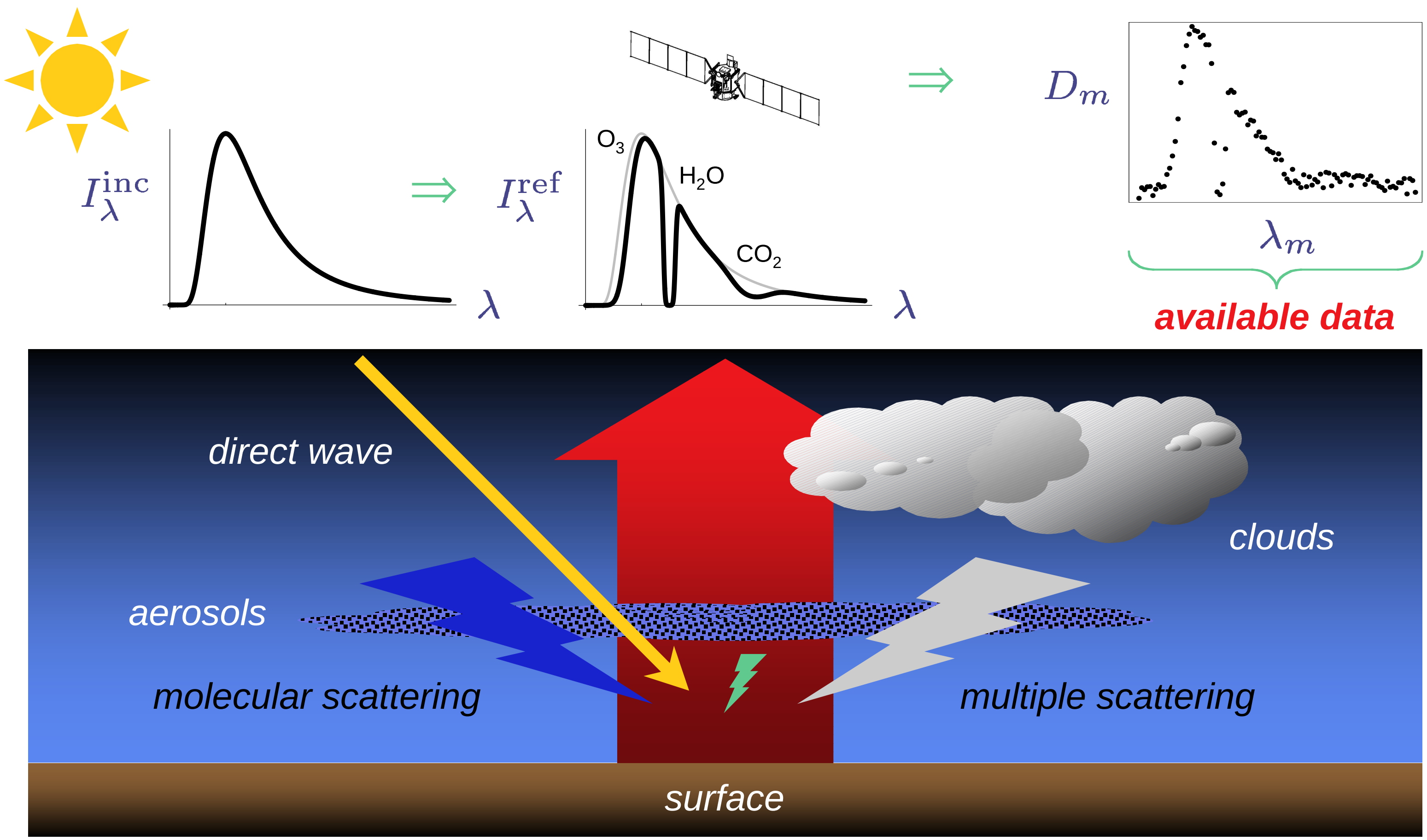
- The canonical remote-sensing problem
- Elements of Bayesian inference
- Forward model for a gaseous atmosphere
  - light–matter interactions
  - radiative transfer in an extended medium
- The joint (atmospheric **and** surface) retrieval problem
  - state of the practice in hyperspectral processing
  - present work

as time permits

- Forward model for an electro-optic sensor (abridged from talk at IGARSS – Toulouse, France, July 2003)

The remote-sensing problem

- Hyperspectral (satellite) remote-sensing scenario



Bayesian data-analysis framework

- Bayes' theorem – datum D, parameter x

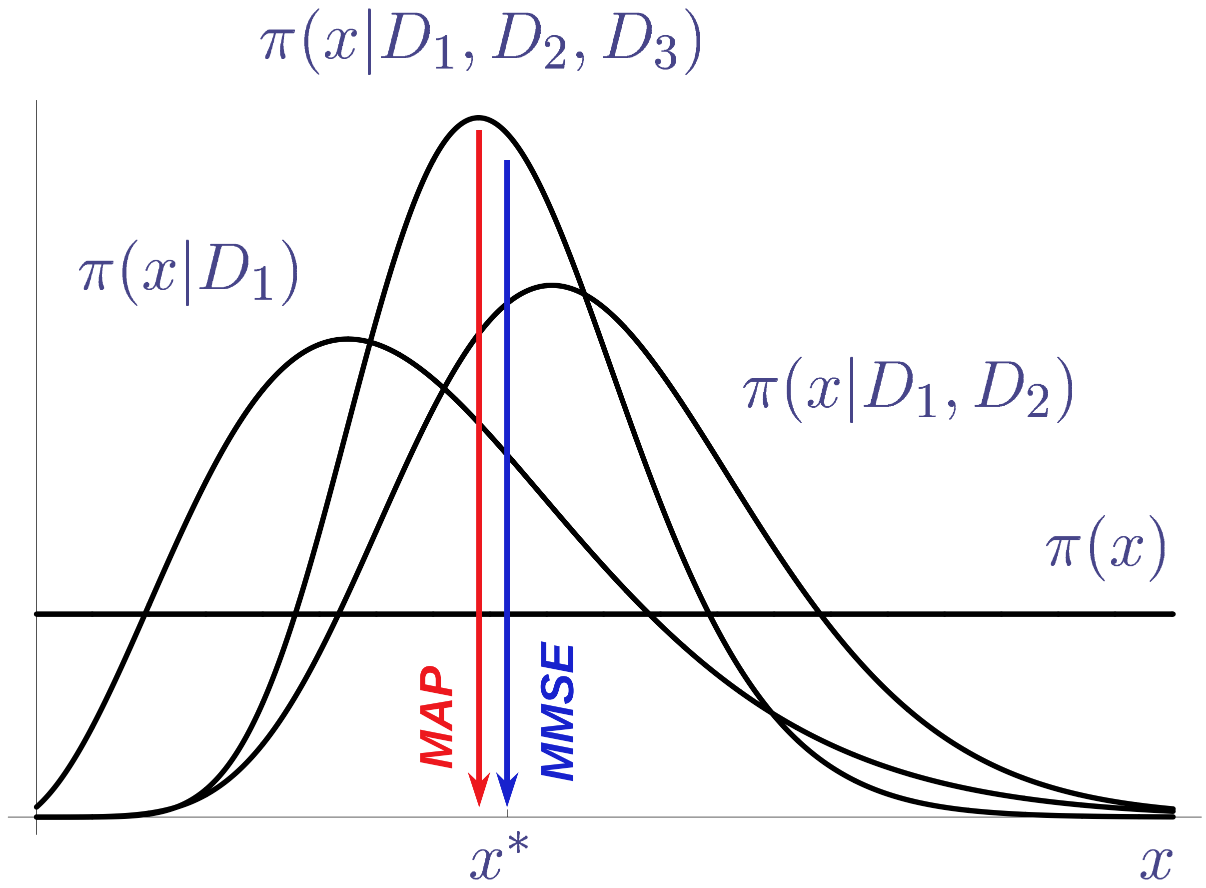
$$\pi(x|D) = \frac{\ell(D|x)\,\pi(x)}{\int \ell(D|x)\,\pi(x)\,\mathrm{d}x} = \frac{likelihood \cdot prior}{evidence} = posterior$$

- Generalization
  - multiple independent measurements
    $\mathcal{D} = \{D_m, m = 1, 2, \ldots, M\}$
  - multiple unknown parameters
    $\mathcal{X} = \{x_n, n = 1, 2, \ldots, N\}$

$$\pi(\mathcal{X}|\mathcal{D}) = \frac{\ell(\mathcal{D}|\mathcal{X})\,\pi(\mathcal{X})}{\pi(\mathcal{D})} \propto \pi(\mathcal{X}) \prod_{m=1}^{M} \ell(D_m|\mathcal{X})$$

Bayesian learning

- Data leading to improved state of knowledge about x:



Bayesian inference (or “retrieval”)

- Maximum *a posteriori* estimate:

$$\left.\frac{\partial \pi(x|\mathcal{D})}{\partial x}\right|_{x^*} = 0, \qquad \left.\frac{\partial^2 \pi(x|\mathcal{D})}{\partial x^2}\right|_{x^*} < 0$$

  - optimization methods: simulated annealing, Gauss–Newton, Levenberg–Marquardt, *etc.*

- Minimum mean-squared error estimate:

$$x^* = \langle x \rangle = \int x\, \pi(x|\mathcal{D})\, \mathrm{d}x, \qquad \sigma_x^2 = \int (x - x^*)^2\, \pi(x|\mathcal{D})\, \mathrm{d}x$$

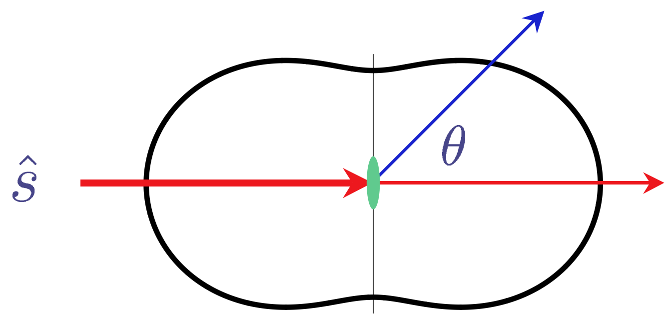
  - integration methods: Markov-chain Monte Carlo

- Computational challenge: $N = \dim \mathcal{X} \sim \mathcal{O}(10^2)$

Unperturbed light–matter interaction

- Unpolarized light incident on a stationary molecule

scattering $\quad p_\nu = \frac{3}{4}\left(1+\cos^2\theta\right), \qquad C_\nu^{\mathrm{sca}} = \frac{k_0^4}{6\pi\epsilon_0^2}\,|\gamma_\nu|^2$

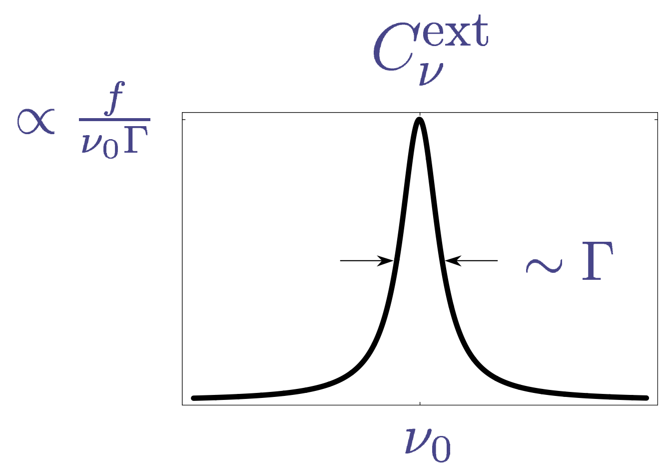


$$C_\nu^{\mathrm{ext}} = C_\nu^{\mathrm{sca}} + C_\nu^{\mathrm{abs}} = \frac{k_0}{\epsilon_0}\,\Im\{\gamma_\nu\}$$

extinction

polarizability

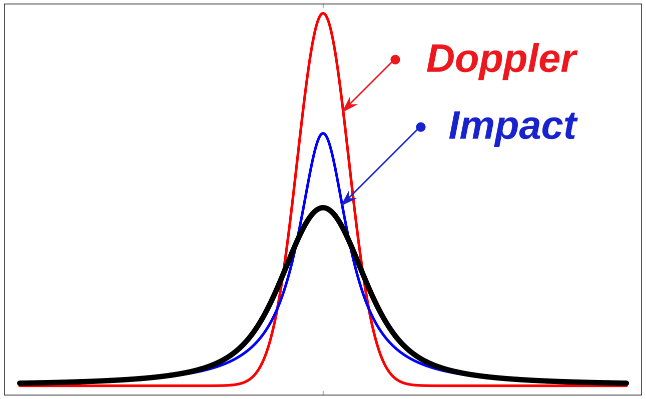
$$\gamma_\nu = \frac{e^2}{m}\sum_j \frac{f_j}{\nu_{0j}^2-\nu^2-i\nu\Gamma_j}$$



Perturbed light–matter interaction

- Temperature and pressure broadening: the Voigt line

$$\phi(\nu - \nu_0)$$



$$\nu_0$$

$$\phi(\nu - \nu_0; \Gamma_\mathrm{D}, \Gamma_\mathrm{I}) = \frac{1}{\sqrt{\pi}\,\Gamma_\mathrm{D}}\, K\left(\frac{\nu-\nu_0}{\Gamma_\mathrm{D}}, \frac{\Gamma_\mathrm{I}}{\Gamma_\mathrm{D}}\right)$$

$$K(x,y) \equiv \frac{y}{\pi} \int_{-\infty}^{\infty} \frac{\mathrm{e}^{-t^2}}{(x-t)^2+y^2}\,\mathrm{d}t$$

- Extinction cross section of an inhomogeneous gas

$$C_\nu^\mathrm{ext}(\vec{r}) = \sum_j S_j[T(\vec{r})]\,\phi\{\nu - \nu_{0j}; \Gamma_{\mathrm{D}j}[T(\vec{r})], \Gamma_{\mathrm{I}j}[p(\vec{r}), T(\vec{r})]\}$$
$$+ \kappa_\nu^\mathrm{con}(\vec{r})$$

Optics of a gaseous atmosphere

- Spatial molecular number density of the i^{th} gas $n_i(\vec{r})$
- Scattering and extinction coefficients of the medium

$$\sigma_\nu(\vec{r}) = \sum_i C_{i\nu}^{\text{sca}}(\vec{r})\, n_i(\vec{r}), \qquad \kappa_\nu(\vec{r}) = \sum_i C_{i\nu}^{\text{ext}}(\vec{r})\, n_i(\vec{r})$$

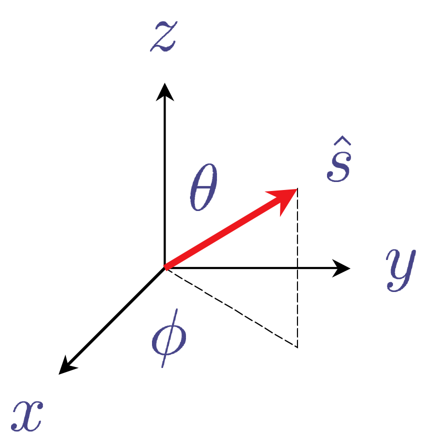
- Radiation field as a "photon gas" with intensity $I_\nu(\vec{r}, \hat{s})$

$$\hat{s} \cdot \vec{\nabla} I_\nu(\vec{r}, \hat{s}) = - \underbrace{\kappa_\nu(\vec{r})\, I_\nu(\vec{r}, \hat{s})}_{\text{rate of extinction}} + \underbrace{\sigma_\nu(\vec{r}) \int_{4\pi} p_\nu(\vec{r}, \hat{s}; \hat{s}')\, I_\nu(\vec{r}, \hat{s}')\, \frac{\mathrm{d}\hat{s}'}{4\pi}}_{\text{source function}}$$

Atmospheric radiative transfer

- Vertically-stratified (*i.e.*, plane-parallel) atmosphere
  - DISORT code, HITRAN database, Kurucz spectrum

$$\mu \frac{\mathrm{d}I_\nu}{\mathrm{d}\tau} = I_\nu(\tau,\Omega) - \varpi_\nu(\tau) \int_{4\pi} p_\nu(\tau,\Omega;\Omega')\, I_\nu(\tau,\Omega')\, \frac{\mathrm{d}\Omega'}{4\pi}$$



$$\mu \equiv \cos\theta, \qquad \varpi_\nu \equiv \tfrac{\sigma_\nu}{\kappa_\nu} = \tfrac{\sigma_\nu}{\sigma_\nu+\alpha_\nu}$$

$$\tau_\nu(z) \equiv \textstyle\int_z^\infty \kappa_\nu(\zeta)\,\mathrm{d}\zeta, \qquad \tau^* = \tau_\nu(0)$$

boundary conditions

$$I_\nu^-(0,\Omega) = F_\nu^{\mathrm{s}}\,\delta(\mu+\mu^{\mathrm{s}})\,\delta(\phi-\pi-\phi^{\mathrm{s}})$$

$$I_\nu^+(\tau^*,\Omega) = \textstyle\int_{2\pi} \rho_\nu(\Omega;\Omega')\, I_\nu^-(\tau^*,\Omega')\mathrm{d}\Omega'$$

The retrieval problem

- Atmospheric and surface “state” parameters
  - vertical temperature and pressure profiles
  - vertical trace-gas concentration profiles
  - surface spectral BRDF

$$\mathcal{X} = \{\vec{T}, \vec{p}, \vec{n}_i, \vec{\rho}\}, \quad \vec{v} \equiv \{v(z_l), l = 1, 2, \ldots, L\}$$

- Computational challenge: 4 nested loops!

`for i = 1 to` $\mathcal{O}(10)$	gases
`for j = 1 to` $\mathcal{O}(10^4)$	lines
`for k = 1 to` $\mathcal{O}(10)$	spectral points
`for l = 1 to` $\mathcal{O}(10)$	vertical layers

State of the practice

Context: hyperspectral imager *Hyperion* (see June 2003 Special Issue of *IEEE Trans. Geoscience and Remote Sensing*

- Atmosphere regarded as a “nuisance”
- Forward models unsuitable for dynamic (Bayesian) inference
  - best fit to pre-computed look-up tables:
    - vertical profiles from 1976 US Standard Atmospheres
    - correlated-k method for band-averaged optical depths
- Spectral and spatial image information content largely unused, or handled by clustering, PCA, *etc.*!

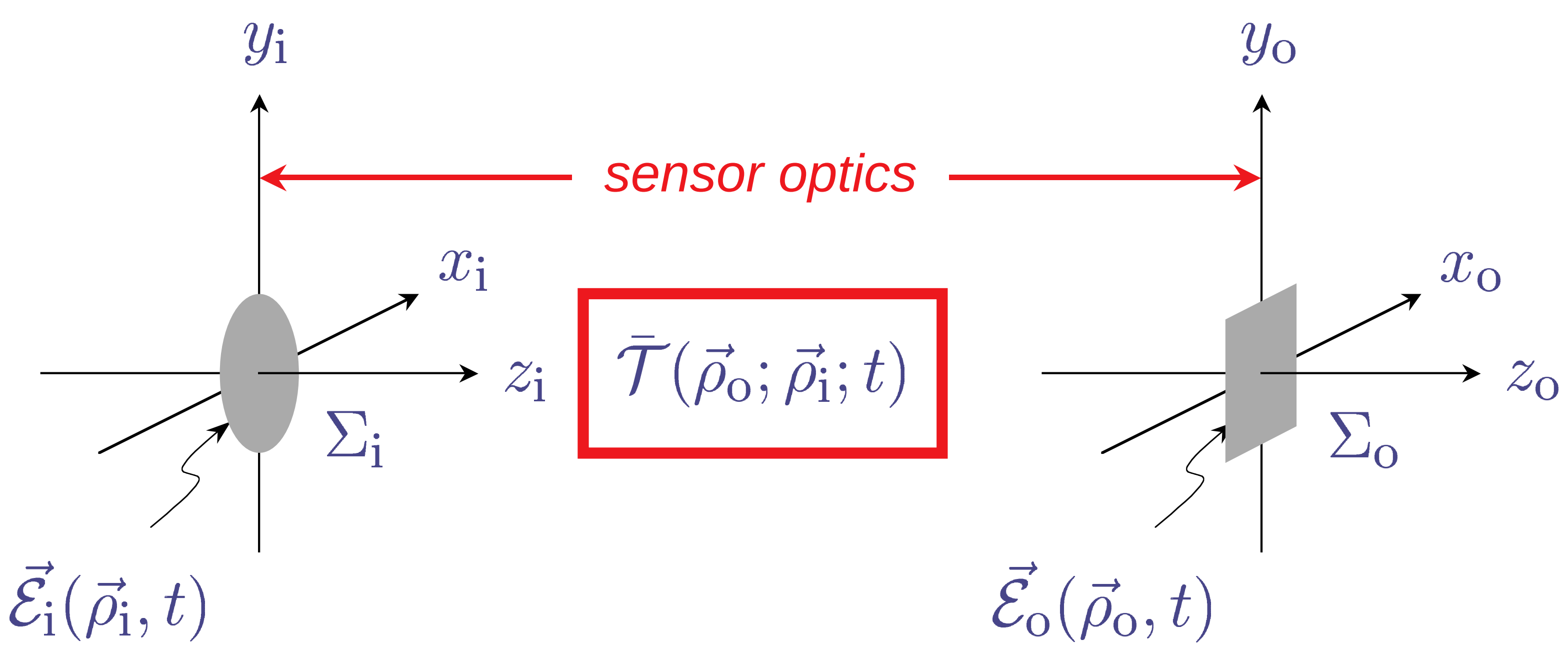
Present work

- Atmosphere jointly inferred along with the surface
- Efficient **and** accurate forward model:
  - new approach to the handling of the continuum
  - FFT-based Voigt calculation
  - linearised DISORT (see Spurr *et al.* in *JQSRT*, 2002)
  - semi-analytical Jacobians
  - vectorial DISORT *coming soon*
- Spectral and spatial (Markovian) covariance structure learned via hierarchical Bayesian inference
- “Ground-truth” data from DOE ARM site campaign archives, coincident in space and time with *Hyperion* data

Optical subsystem

- Linear, time-invariant, space-varying impulse response
  - $\bar{\mathcal{T}} = 0$ for $t < 0$, $\vec{\rho}_{\mathrm{i}} \notin \Sigma_{\mathrm{i}}$, or $\vec{\rho}_{\mathrm{o}} \notin \Sigma_{\mathrm{o}}$

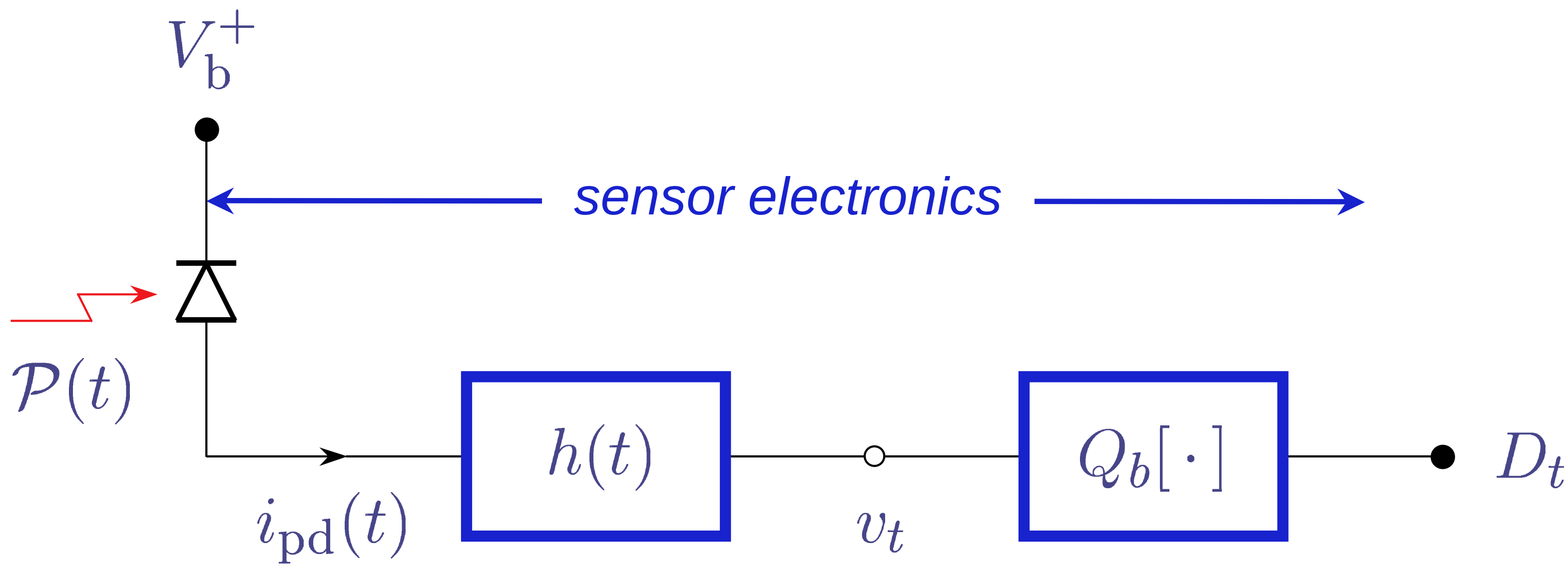
$$\vec{\mathcal{E}}_{\mathrm{o}}(\vec{\rho}_{\mathrm{o}}, t) = \int_{-\infty}^{\infty} \iint_{-\infty}^{\infty} \bar{\mathcal{T}}(\vec{\rho}_{\mathrm{o}}; \vec{\rho}_{\mathrm{i}}; t - t') \cdot \vec{\mathcal{E}}_{\mathrm{i}}(\vec{\rho}_{\mathrm{i}}, t')\, \mathrm{d}^2\vec{\rho}_{\mathrm{i}}\, \mathrm{d}t'$$



Electrical subsystem

- Continuous output v_t; (b-bit) discrete output D_t

$$v_t = \sum_{k=1}^{K} h(t - t_k) + \left[\sum_{l=1}^{L} h(t - t_l) + \xi(t) \right] = signal + noise$$



Signal statistics

- Output signal voltage
  - filtered, doubly-stochastic Poisson process

$$v_t^{\mathrm{s}} \equiv \sum_{k=1}^{K} h(t - t_k)$$

- Characteristic function
  - stochastic photoelectron rate process $r(t)$
  - analog-to-digital converter integration time T_*

$$\Phi^{\mathrm{s}}(u) = \mathbb{E}\left\{ \exp\left(\int_{t-T_*}^{t} r(t') \left[\mathrm{e}^{\mathrm{i}uh(t-t')} - 1 \right] \mathrm{d}t' \right) \right\}$$

The rate process

- Detected power $\mathcal{P}(t)$ normalized by photon energy

$$r(t) = \frac{1}{(2\pi)^4} \iint_{-\infty}^{\infty} \frac{1}{\hbar|\omega|}\, \mathrm{e}^{-\mathrm{i}(\omega-\omega')t} \cdot \iint_{-\infty}^{\infty} \mathsf{E}_{\mathrm{o}}^{T}(\vec{k}_{\mathrm{o}},\omega)\, \mathsf{Q}^{*}(\vec{k}_{\mathrm{o}},\omega')\, \mathsf{E}_{\mathrm{o}}^{*}(\vec{k}_{\mathrm{o}},\omega')\, \mathrm{d}^2\vec{k}_{\mathrm{o}}\, \mathrm{d}\omega\, \mathrm{d}\omega'$$

- Narrow-band optical system – center frequency ω_{c}

$$\mathsf{T}(\vec{k}_{\mathrm{o}};\vec{k}_{\mathrm{i}};\omega) = \frac{1}{2}\mathsf{H}(\vec{k}_{\mathrm{o}};\vec{k}_{\mathrm{i}};\omega-\omega_{\mathrm{c}}) + \mathrm{c.\,s.}$$

$$\mathsf{E}_{\mathrm{o}}(\vec{k}_{\mathrm{o}},\omega) = \frac{1}{(2\pi)^2} \iint_{-\infty}^{\infty} \mathsf{T}(\vec{k}_{\mathrm{o}};\vec{k}_{\mathrm{i}};\omega)\, \mathsf{E}_{\mathrm{i}}(\vec{k}_{\mathrm{i}},\omega)\, \mathrm{d}^2\vec{k}_{\mathrm{i}}$$

Noise statistics

- Output noise voltage
  - Photodiode dark-noise current
    - filtered, homogeneous Poisson process – rate ρ
  - Amplifier & ADC thermal-noise voltage
    - zero-mean Gaussian process – variance σ_T^2

$$v_t^{\mathrm{n}} \equiv \sum_{l=1}^{L} h(t - t_l) + \xi(t)$$

- Characteristic function

$$\Phi^{\mathrm{n}}(u) = \exp\left(\rho \int_0^{T_*} \left[\mathrm{e}^{\mathrm{i}uh(t')} - 1\right] \mathrm{d}t' - \frac{1}{2}\sigma_T^2 u^2\right)$$

Continuous output

- “Photon-counting” approximation

$$h(t) \simeq \gamma\, e \equiv \Gamma, \quad 0 \leq t \leq T_*$$

- Integrated intensity

$$w(t) \equiv \int_{t-T_*}^{t} r(t')\,\mathrm{d}t'$$

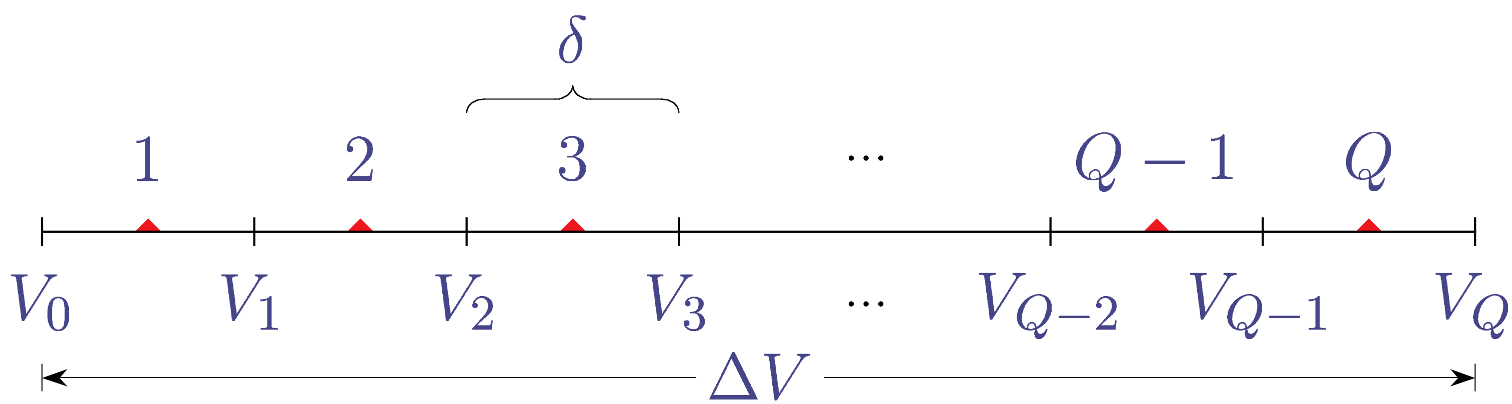
- Output characteristic function

$$\begin{aligned}\Phi(u) &= \Phi^{\mathrm{s}}(u)\,\Phi^{\mathrm{n}}(u)\\ &\simeq \Phi_w\left[\mathrm{i}\left(1-\mathrm{e}^{\mathrm{i}\Gamma u}\right)\right]\,\exp\left[\rho\,T_*\left(\mathrm{e}^{\mathrm{i}\Gamma u}-1\right)-\frac{1}{2}\sigma_T^2 u^2\right]\end{aligned}$$

Discrete output

- Probability density of the discrete output D_t
  - $Q = 2^b$, $q = 1, 2, \ldots, Q$, $\delta = \frac{\Delta V}{Q}$

$$P_q \equiv P\{D_t = q\} = \frac{\delta}{2\pi} \int_{-\infty}^{\infty} \Phi(u) \operatorname{sinc}\left(\frac{\delta u}{2\pi}\right) \mathrm{e}^{-\mathrm{i}uq} \,\mathrm{d}u$$



Output statistics

- Edgeworth (a.k.a. Gram–Charlier) series

$$P_q = \frac{\delta}{\sqrt{2\pi}\sigma} \exp\left[-\left(\frac{q-\eta}{\sqrt{2}\sigma}\right)^2\right]\left[1+\sum_{r=3}^{\infty}\frac{\kappa_r}{r!}H_r\left(\frac{q-\eta}{\sqrt{2}\sigma}\right)\right]$$

  - parameters – general case, $\delta \ll \sigma$

$$\begin{aligned}
\eta &= \Gamma\left(\bar{w} + \langle\tilde{w}\rangle + \rho\, T_*\right) \\
\sigma^2 &= \Gamma\,\eta + \Gamma^2\left(2\bar{w} + \langle\tilde{w}\rangle\right)\frac{\langle\tilde{w}\rangle}{\mathcal{M}} + \sigma_T^2 + \frac{\delta^2}{12} \\
\kappa_3 &= \Gamma^2\,\eta + \Gamma^3\left[3\left(2\bar{w} + \langle\tilde{w}\rangle\right) + 2\left(3\bar{w} + \langle\tilde{w}\rangle\right)\frac{\langle\tilde{w}\rangle}{\mathcal{M}}\right]\frac{\langle\tilde{w}\rangle}{\mathcal{M}}
\end{aligned}$$

$\ldots$

Thermal source

- Wide-band, unpolarized source, normal incidence at d

$$\mathsf{E}_\mathrm{i}(\vec{k}_\mathrm{i},\omega) = \left[\frac{1}{2}\,\mathsf{U}_\mathrm{s}(\vec{k}_\mathrm{i},\omega-\bar{\omega}) + \mathrm{c.\,s.}\right]\,\mathrm{e}^{\mathrm{i}\sqrt{k_0^2(\omega)-k_\mathrm{i}^2}\,d}$$

- Integrated intensity statistics – $w = \tilde{w}$

$$\Phi_w(u) = \left(1 - \mathrm{i}u\frac{\langle\tilde{w}\rangle}{\mathcal{M}}\right)^{-\mathcal{M}}$$

$$\begin{aligned}\langle\tilde{w}\rangle = \frac{T_*}{8}\,\frac{1}{(2\pi)^7}\int_{-\infty}^{\infty}\mathrm{d}\omega\,\frac{1}{\hbar|\omega|}\int\cdots\int_{-\infty}^{\infty}\mathrm{d}^2\vec{k}_\mathrm{i}\,\mathrm{d}^2\vec{k}'_\mathrm{i}\,\mathrm{d}^2\vec{k}_\mathrm{o}\\ \cdot\left\{\mathsf{H}^T(\vec{k}_\mathrm{o};\vec{k}_\mathrm{i};\omega-\omega_\mathrm{c})\,\mathsf{Q}^*(\vec{k}_\mathrm{o},\omega)\,\mathsf{H}^*(\vec{k}_\mathrm{o};\vec{k}'_\mathrm{i};\omega-\omega_\mathrm{c})\right\}_{11+22}\\ \cdot\,G_\mathrm{s}(\vec{k}_\mathrm{i};\vec{k}'_\mathrm{i};\omega)\,\mathrm{e}^{\mathrm{i}\left[\sqrt{k_0^2(\omega)-k_\mathrm{i}^2}-\sqrt{k_0^2(\omega)-k_\mathrm{i}'^2}\right]d}\end{aligned}$$

Laser source

- Narrow-band, (x-)polarized, collimated source

$$E_{\mathrm{i}x}(\vec{k}_{\mathrm{i}},\omega) = \frac{(2\pi)^2}{2}\,\delta(\vec{k}_{\mathrm{i}}-\vec{k}_{\mathrm{s}})\left[2\pi\,\bar{U}_{\mathrm{s}}\,\delta(\omega-\bar{\omega}) + \tilde{U}_{\mathrm{s}}(\omega-\bar{\omega})\right] + \mathrm{c.\,s.}$$

- Integrated intensity statistics – $w = \bar{w} + \tilde{w}$

$$\Phi_w(u) = \left(1 - \mathrm{i}u\frac{\langle\tilde{w}\rangle}{\mathcal{M}}\right)^{-\mathcal{M}} \exp\left(\frac{\mathrm{i}u\bar{w}}{1-\mathrm{i}u\frac{\langle\tilde{w}\rangle}{\mathcal{M}}}\right)$$

$$\bar{w} = \frac{T_*}{8}\,\frac{|\bar{U}_{\mathrm{s}}|^2}{\hbar|\omega|}\int\!\!\int_{-\infty}^{\infty} \mathrm{d}^2\vec{k}_{\mathrm{o}} \cdot \left\{ \mathsf{H}^T(\vec{k}_{\mathrm{o}};\vec{k}_{\mathrm{s}};\bar{\omega}-\omega_{\mathrm{c}})\,\mathsf{Q}^*(\vec{k}_{\mathrm{o}},\bar{\omega})\,\mathsf{H}^*(\vec{k}_{\mathrm{o}};\vec{k}_{\mathrm{s}};\bar{\omega}-\omega_{\mathrm{c}}) \right\}_{11}$$